Multiscale Characterization of bcc Crystals Deformed to Large Extents of Strain

Experimental data is crucial in the process of constructing and validating the multiscale crystal plasticity models used in computer code simulations of materials deformed under extreme conditions, such as high strain rate, high pressure, and large extents of strain. The "6 Degrees of Freedom" (6DOF) experiment was designed specifically for this task and has provided data on the behavior of bcc crystals that may revolutionize the field.

Until now, the experimental data and simulation efforts have focused on relatively small extents of plastic deformation (0.5%). Both experiments and modeling must now be extended to large strain deformations on the order of tens of percent. At these larger extents of strain, the use of multiscale characterization tools can be improved to better understand the fundamental behavior.

Project Goals

Our goal is to develop large strain experiments that will provide the essential data to enhance LLNL's multiscale modeling capability through the validation of dislocation dynamics (DD) simulations and the construction of continuum strength models.

Relevance to LLNL Mission

Understanding and simulating the plastic, or non-reversible, deformation of body-centered cubic (bcc) metals, is a major component of LLNL's Stockpile Stewardship Program and will be used to simulate future NIF experiments.

FY2005 Accomplishments and Results

Experimental technique and large strain data. Using the accomplishments from FY2004, a full-field 3-D image correlation strain measurement system that compares sequential photos to determine the local movement of spots has been incorporated into the 6DOF experiment. Unlike traditional testing techniques, ours allows essentially unconstrained deformation of the crystal. Figure 1 shows results from an experiment on a zinc single crystal, performed to verify the accuracy of the 6DOF experiment and highlight the use of the image correlation method.

A major challenge in conducting experiments to large strains is that due to the anisotropic nature of the deformation, or slip, of a single crystal, a severe shape change can develop, which can lead to errors in the analysis and development of the models. To

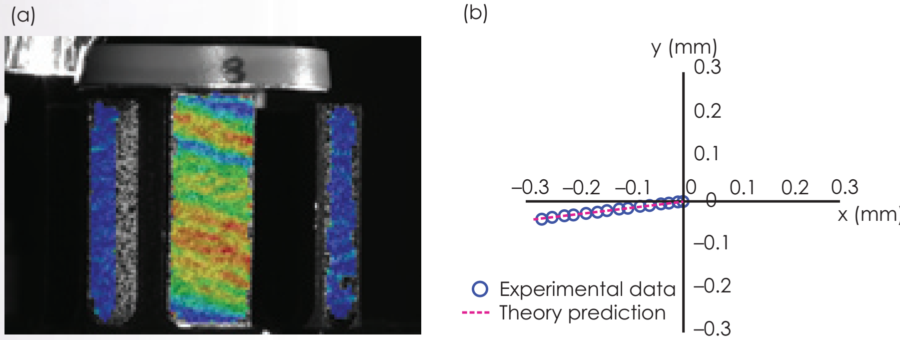
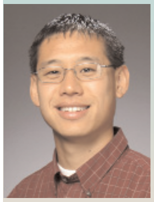


Figure 1. Zinc experiment validating the 6DOF experiment. (a) Image correlation strain map superimposed onto the sample. (b) Translation of the bottom of the sample, which matches exactly with theoretical predictions.



For more information contact
Jeffrey Florando
(925) 422-0698
florando1@llnl.gov

combat this issue, samples can be remachined to maintain a nominally uniform shape. A molybdenum (Mo) sample (bcc structure), which was previously deformed to 2.5% strain, has been remachined and deformed an additional 2.5%, for a total of 5% strain. The corresponding stress-strain curve and translation of the sample (Fig. 2) show that the underlying deformation mechanisms are similar before and after remachining, and are still significantly different from predictions of conventional theories.

Characterization of the deformed material. One method of characterizing the deformed material is using the x-ray microdiffraction beamline at the Advanced Light Source at Lawrence Berkeley National Laboratory. The high-energy synchrotron light source allows the analysis of subsurface dislocation structure. This technique can detect features over an area larger than that using transmission electron microscopy (TEM). Results on deformed Mo samples show streaking of the x-ray spots (Fig. 3), indicating considerable deformation on the anomalous plane and confirming the 6DOF compression results.

Connection between experiments and simulations. In a coordinated effort with the dislocation dynamics (DD) simulation development team, the underlying physics of high-temperature deformation of bcc metals is being investigated. Large strain experiments on symmetrically oriented samples, [001] and [110], at 500 K have been performed. Both the experimental and the DD results show a large difference in the strain hardening rate between the [001] and [110] samples. This orientation dependence can be explained with four-node junctions, which is an effect first seen in the DD code and verified experimentally.

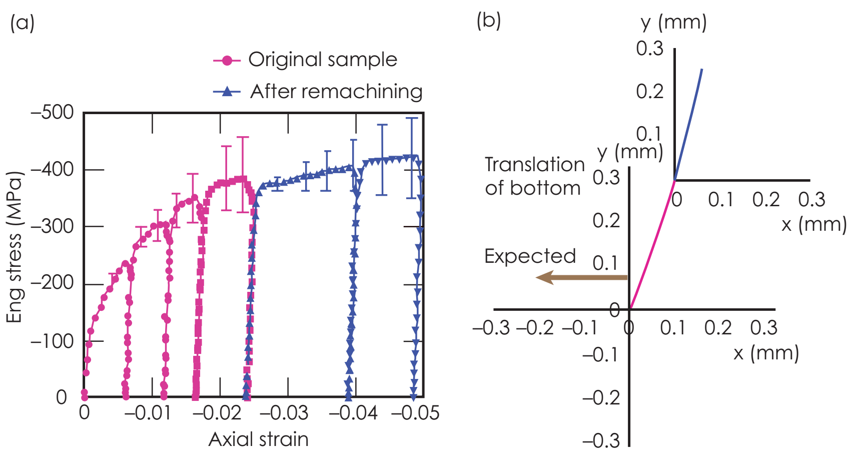


Figure 2. Experimental results on Mo sample before and after remachining. (a) Stress-strain curve showing behavior out to 5% strain. (b) Translation of the bottom of the sample, inconsistent with theoretical predictions.

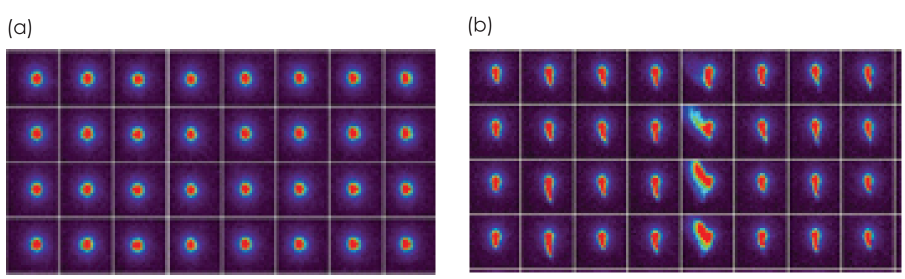


Figure 3. X-ray microdiffraction results on deformed Mo sample (011) plane. Each spot represents a 2-μm area; the spacing between spots is 3 μm. (a) Undeformed sample showing round spots. (b) Deformed sample showing extensive streaking.

Related References

1. Lassila, D.H., M. M. LeBlanc, and G. J. Kay, "Uniaxial Stress Deformation Experiments for Validation of 3-D Dislocation Dynamics Simulations," *J. Eng. Mat. Tech.*, **124**, p. 290, 2002.
2. Bulatov, V. V., and W. Cai, "Nodal Effects in Dislocation Mobility," *Phys. Review Letters*, **89**, p. 115501-1, 2000.

FY2006 Proposed Work

Asymmetric-oriented Mo samples will continue to be remachined to achieve strain values out to 15%. The deformed samples will be characterized using x-ray microdiffraction and TEM to study the evolution of the dislocation structure. New theories that might explain the experimentally observed anomalous behavior will be implemented into the DD code. Experiments on Mo single crystals of different orientations will be conducted for comparison with the new theories.